Computational Mathematics

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Dr. Fariba Fahroo
Program Manager
AFOSR/RSL
Air Force Research Laboratory

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NAME: **Fariba Fahroo**

BRIEF DESCRIPTION OF PORTFOLIO:

Discover Mathematical Algorithms and Develop Computational Techniques that Provide More **Accurate**, **Reliable**, and **Efficient** Algorithms for Modeling and Simulation and Design of Complex Systems for the U.S. Air Force with radical cost and turn-time improvements.

LIST SUB-AREAS IN PORTFOLIO:

- ***Multi-Scale Modeling (plasma, structures, fluids, combustion)***
- ***Multi-Physics Modeling (fluid-structure interactions, particle-fluid models)***
- ***Uncertainty Quantification***
- ***Multidisciplinary Optimization and Control (Design Under Uncertainty)***

Transformational Opportunities for Computational Math

- The next generation of computing systems based on emerging heterogeneous architectures offer unprecedented capabilities for computational science. ➔ *Predictive High-Fidelity Simulations*
- Increase in computing power isn't everything
- *Challenges* :
  - Constraints on system Power
  - slower growth in Memory bandwidth and capacity,
  - Cost of data movement ,
  - Slower growth in clock rate and move to Concurrency of higher number of nodes and threads,
  - Slower growth in I/O bandwidth,
  - Resiliency and Reliability of the computing systems

Addressing the challenges in Computational Science for these emerging computing systems at these scales (peta, exa) require fundamental paradigm shift in algorithms, software, architecture design.

Challenges in Computational Math
The Role of Mathematics

Goal: Simulation, Analysis and Design of complex systems with radical cost and turn-time improvements --- Need for Accurate, Reliable, and Efficient Algorithms

- Multi-Scale Problems (spatial and temporal) --- Not possible to resolve all scales, so there is need for Modeling and passage of information across scales
- Multi-Physics Problems --- Just coupling individual components won't do --- proper Interface formulation
- High-Dimensional Problems --- the curse of dimensionality won't be mitigated fully by more computing power → more math modeling is needed
- Effect of Uncertainty --- ubiquitous, high-dimensional, if not managed, detrimental to accurate analysis and design
- Effect of mesh and geometry --- heart of discretization and algorithms, bad meshes lead to major inaccuracies, need for consideration of complex geometry
- Scalability of Algorithms --- parallelism – New Challenges for emerging architectures

Portfolio's Focus Areas and Outline of Research Highlights

- **Support of High-Order Methods of Accuracy:**
  - **An interplay of Efficiency ,Accuracy and Robustness---- application areas in Structures, Plasma, Combustion**
    - **Highlight of CFD Efforts (2 YIP Projects, AIAA Workshop),**
    - **Transition Stories**
- **Multiscale Methods: Structures**
- **Uncertainty Quantification:**
  - **High-Dimensional Problems**
  - **Bayesian framework for UQ → a MURI 2012 in Material Science**
  - **Design Under Uncertainty → a 2012 BRI topic**

Challenges for High-Order Methods

- Low-order methods suffer from undesirable excessive numerical dissipation, and explicit time-integration methods have severe time-step restrictions for stability for multiscale, multi-physics simulation → need for high-order accurate, implicit methods. BUT
- High-Order methods are not as robust as lower-order ones – convergence to steady-state can stall or be very slow.
- Time- Integration techniques – explicit methods too expensive – need speed-ups in implicit methods (expensive Jacobians in time-integration and preconditioning)
- Robust, compact, accuracy preserving and convergent limiters (for problems with strong discontinuities)
- Low storage, efficient iterative solution methods including hp-multigrid methods for high-order operators → YIP 10 effort exploring sparsity in large expensive Jacobians
- High-order viscous grid generation, error estimate and anisotropic hp-adaptations → YIP 11 effort using adjoint-based, output error methods for adaptation

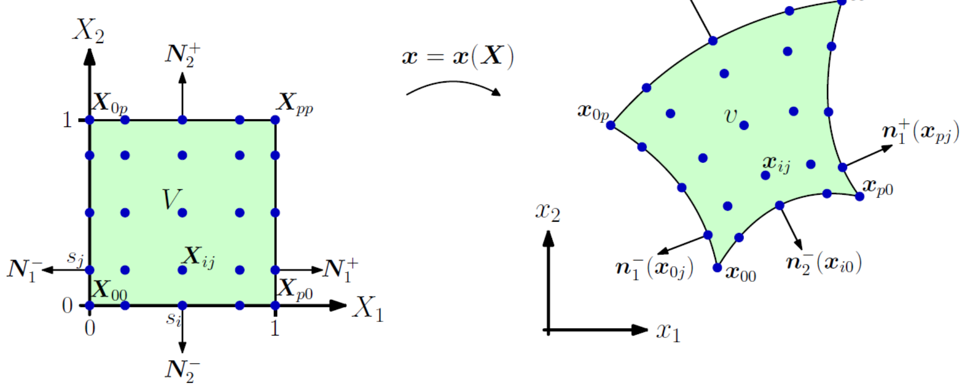
Sparse Line-Based High-Order Methods (Discontinuous Galerkin) on Unstructured Meshes:

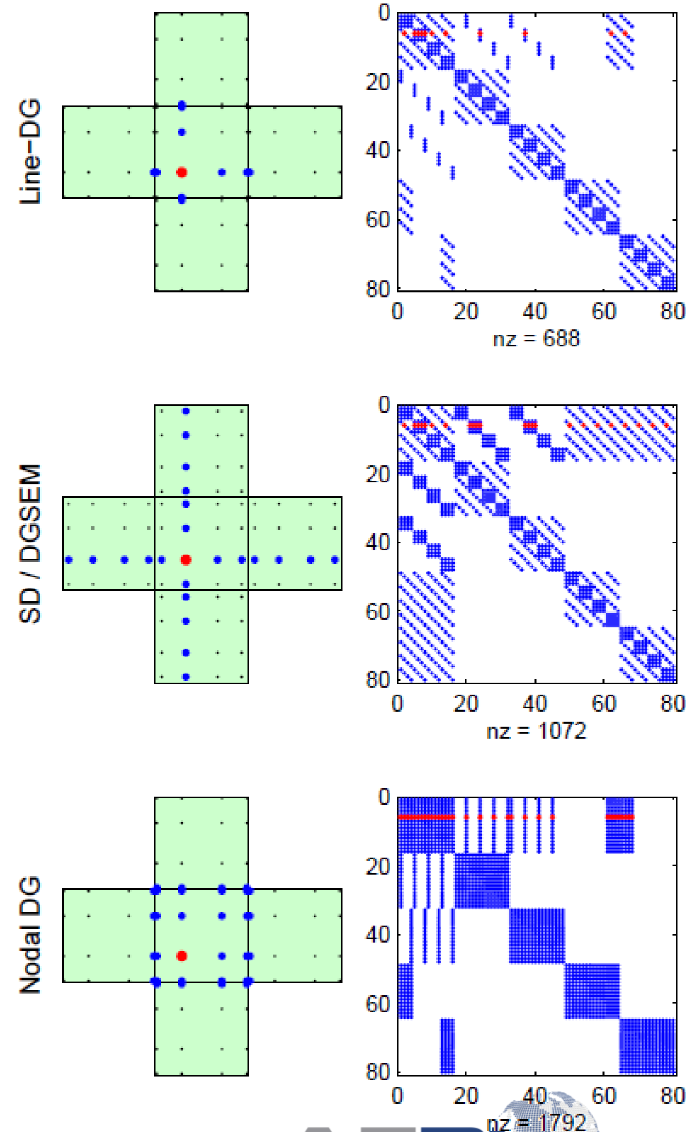
Per-Olof Persson, UC Berkeley (YIP 2010)

Goal: Reduce the cost of implicit solvers by using sparsity in large, expensive jacobians

Line-DG: Apply 1-D DG schemes separately along each coordinate line

- **Magnitudes sparser Jacobians**
- **Simple scheme: Only 1-D integrals**
- **LDG-type second order terms**

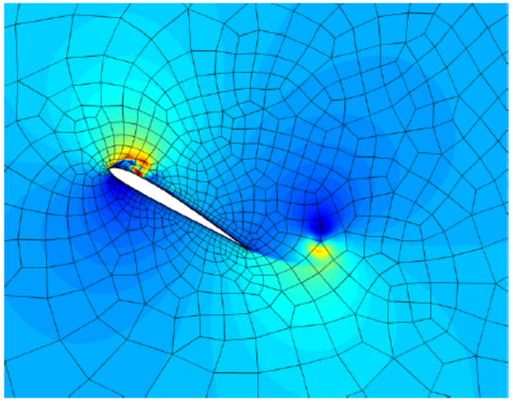


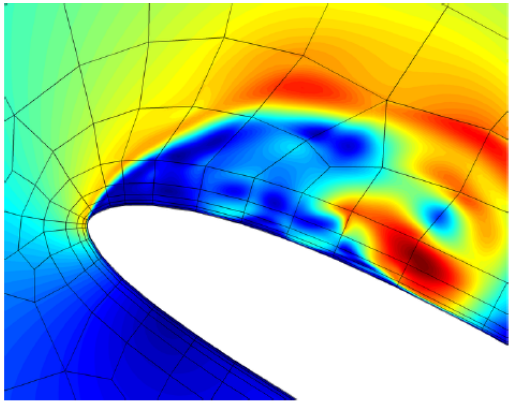


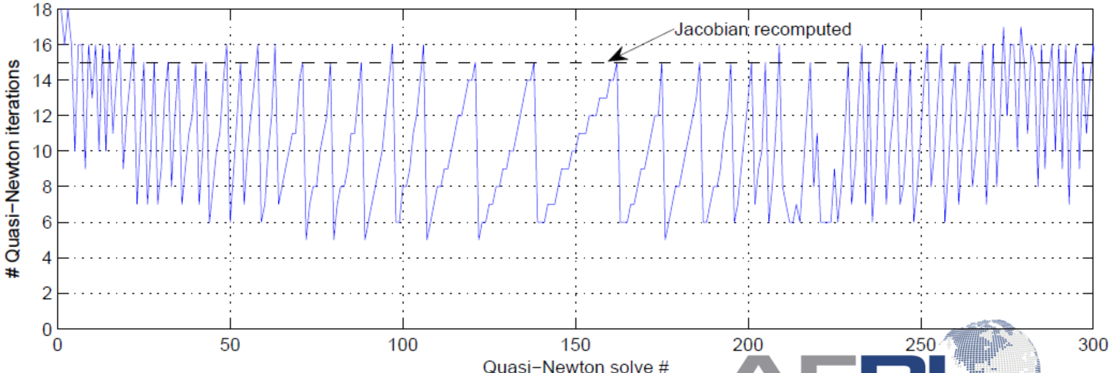
	Polynomial order p	1	2	3	4	5	6	7	8	9	10
2-D	Line-DG connectivities	7	9	11	13	15	17	19	21	23	25
	Spectral Difference connectivities	11	17	23	29	35	41	47	53	59	65
	Nodal-DG connectivities	12	21	32	45	60	77	96	117	140	165
3-D	Line-DG connectivities	10	13	16	19	22	25	28	31	34	37
	Spectral Difference connectivities	16	25	34	43	52	61	70	79	88	97
	Nodal-DG connectivities	32	81	160	275	432	637	896	1215	1600	2057

Sparsity-preserving Quasi-Newton Implicit RK Time-stepping

- **Implicit methods need to solve systems $(I - \alpha \Delta t A)\Delta K_i = G$ with second-order Jacobian matrices $A = K_{11} + K_{12}K_{21}$**
- **Hard-wire GMRES matrix-vector products to retain sparsity**
- **Use quasi-Newton solvers to reduce the number of expensive Jacobian assemblies**
- **Majority of time spent in residual evaluation** ***– an implicit solver for about the same cost as an explicit***







Goal: **Improve robustness and efficiency of unsteady simulations through output-based error estimation and space-time mesh adaptation**

Why Outputs?

Output = scalar quantity computed from the CFD solution

- A CFD solution may contain millions of degrees of freedom
- Often of interest are only a few scalars (forces, moments, etc.)
- It is mathematically easier to speak of "error in an output" than "error in a CFD solution"

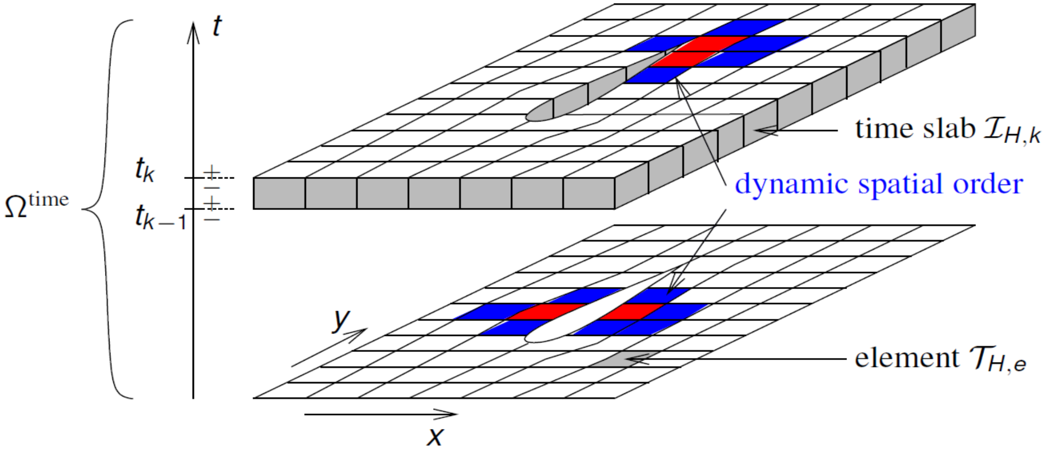
Output error = difference between an output computed with the discrete system solution and that computed with the exact solution to the PDE

Output error estimation

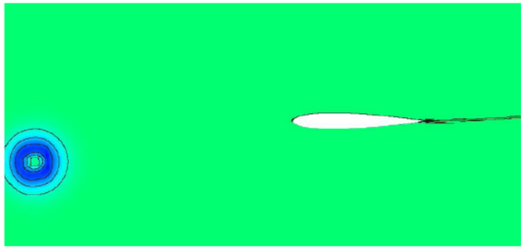
- Identifies all areas of the domain that are important for the accurate prediction of an output
- Accounts for error propagation effects
- Requires solution of an adjoint equation

Variable-Order Adaptation for Unsteady Flows

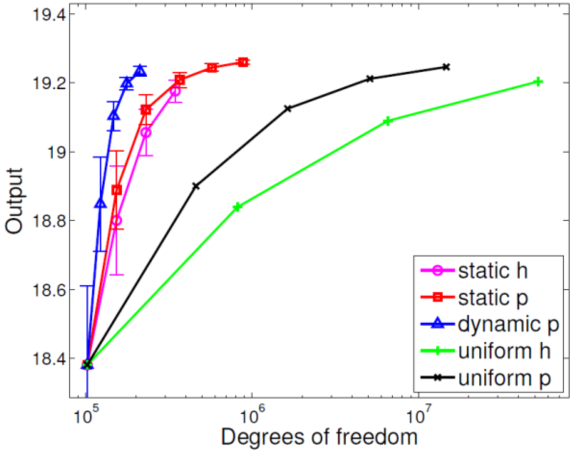
- **Approach:**
- *Discontinuous FEM*
- *Dynamic spatial order refinement*
- *Adjoint-based error estimation*
- *Promising Results but solving adjoint equations is expensive*



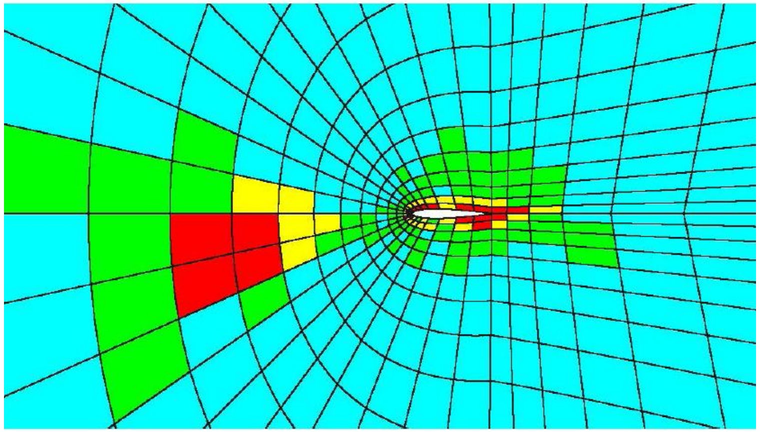
Airfoil-vortex encounter adaptation:



Time integral of airfoil lift coeff

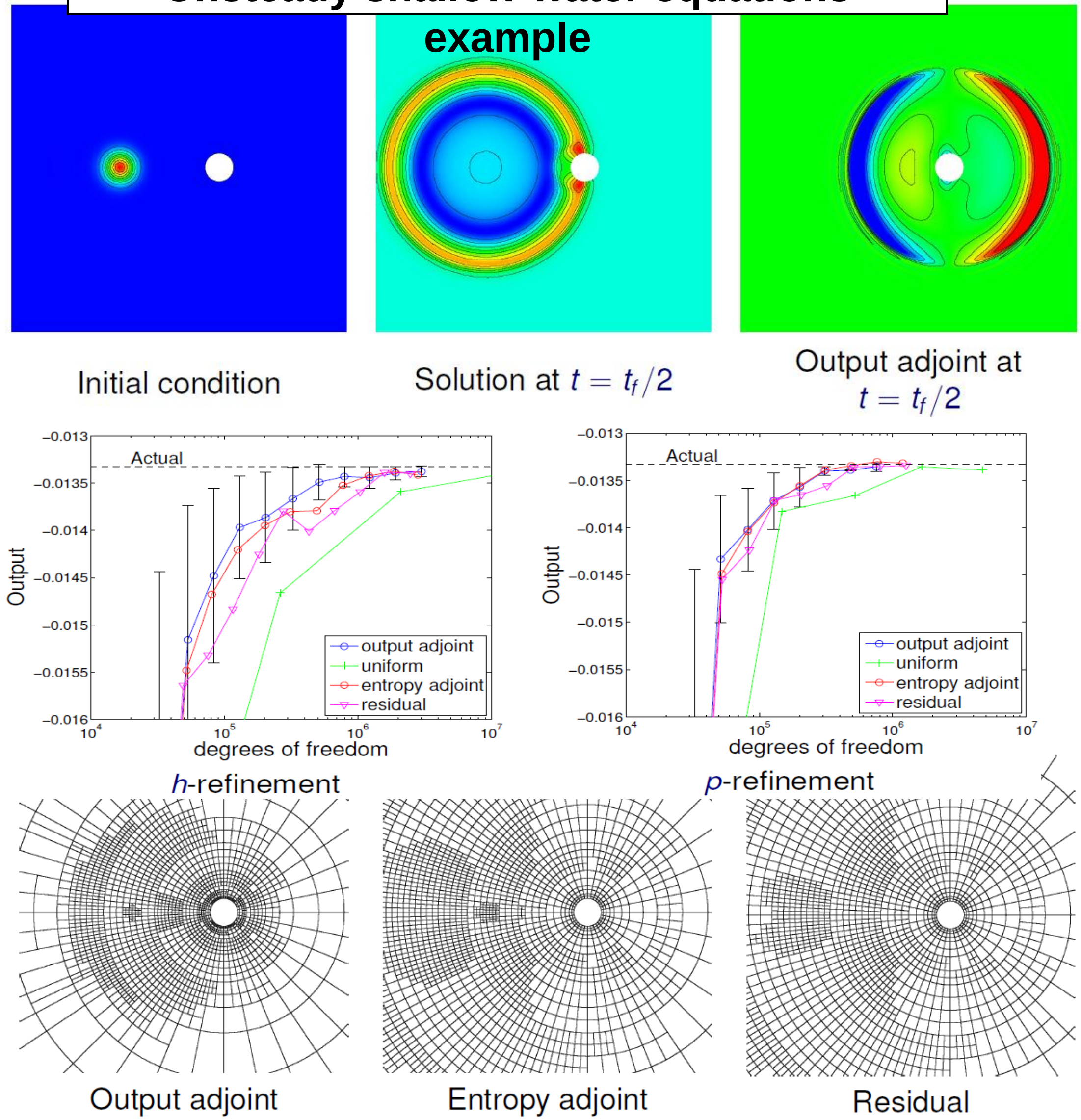


4th adaptive iteration: blue=1, red=5



An Entropy-Adjoint Refinement Indicator

Unsteady shallow-water equations example



Goal: *Analyze properties of a cheap output-based indicator derived from an entropy-adjoint connection*

Approach:

Discontinuous FEM

Steady and unsteady problems

Spatial and temporal refinement

Key Ideas:

Use entropy variables as unsteady adjoint solution for an entropy balance output

Adapting on this output minimizes spurious entropy generation and produces "all-around" good solutions

1st International Workshop on High-Order CFD Methods

- **Workshop held at the 2012 AIAA ASM meeting: a tremendous success**
  - 30 groups from all over the world made over 70 presentations
  - 80 global participants from ~12 countries – 9 PIs
  - Support for students provided by AFOSR

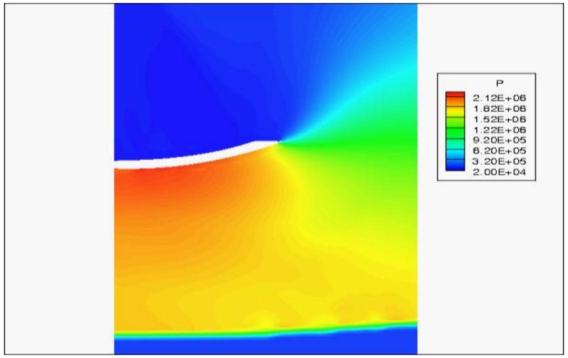
Workshop Summary

- 14 different test cases were considered.
- For smooth inviscid and viscous flow problems, high-order methods outperform 2nd order production codes in terms of error/CPU time
- Solution based grid and accuracy adaptations highly effective in achieving solution efficiency and accuracy
- Further progresses needed for high-order methods to efficiently and robustly solve the Reynolds averaged Navier-stokes equations with turbulence models
- Research on high-order mesh generation with curved boundary is needed
- The 2nd Workshop will be held in Cologne in the summer of 2013

Recent Transitions

- **PI: (Suresh Menon , GA Tech)**
  Hybrid Algorithms for LES of Multi-Phase Flows –Transition to RW

Application to Explosively Formed Projectile (EFP)

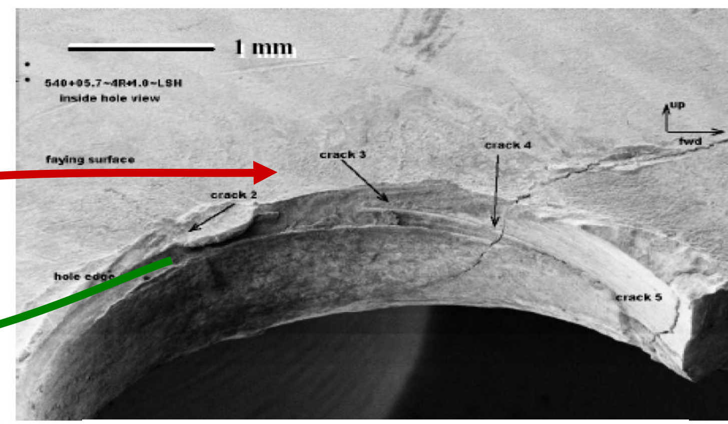


- **PI: (Marsha Berger, NYU)**
  Inclusion of the Adaptation/Adjoint module, Embedded Boundary Methods in the software package Cart3D --- Transition to NASA, ONR, DOE, AFRL, DIA

Cart3D used for computing Formation Flight to reduce drag and improve energy efficiency

A Generalized Finite Element Method for Multiscale Simulations - C.A. Duarte, UIUC

- **Objectives:** Develop and analyze a computational method able to capture multiscale phenomena in structural-scale FEM meshes
- **Approach:** Generalized FEM with global-local enrichment functions: GFEM^{gl}



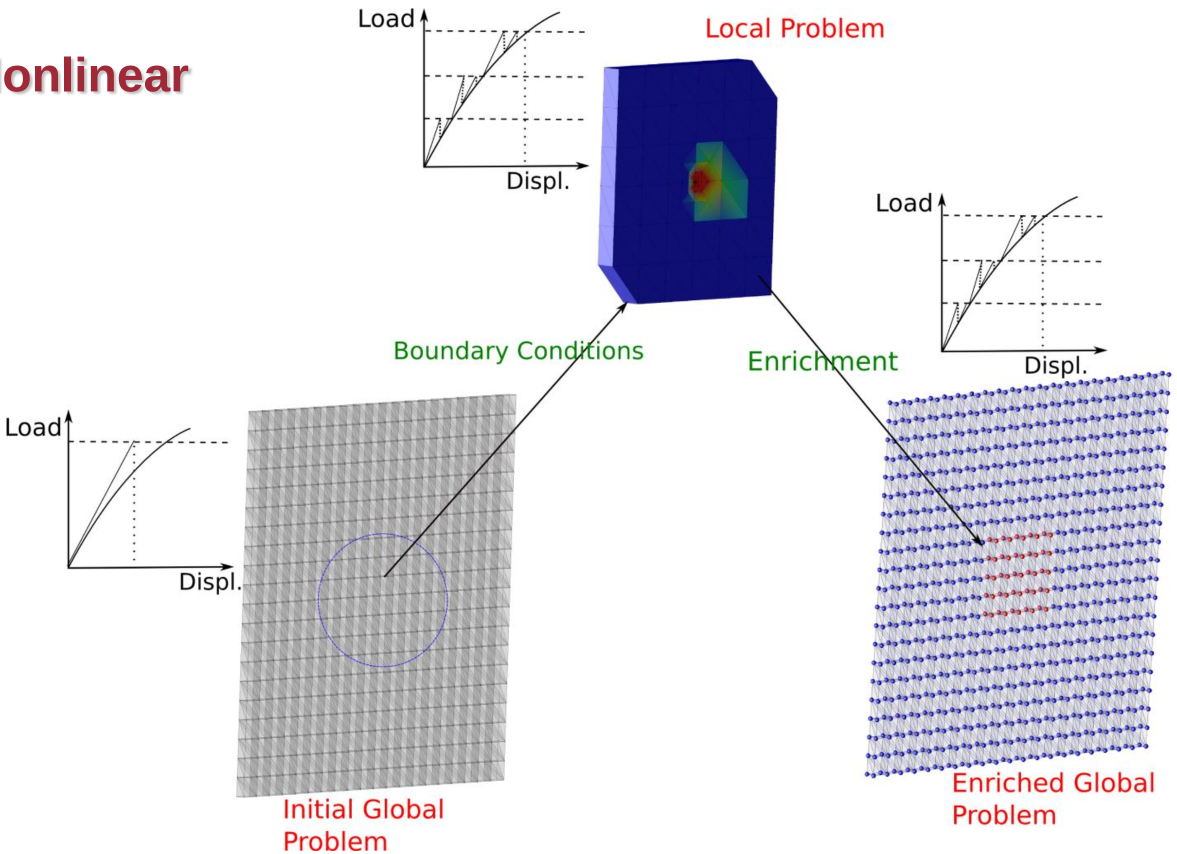
Multiple cracks around a rivet hole

[Sandia National Lab, 2005]

Goal: Capture fine scale effects on *coarse* meshes at the global (structural) scale

A Generalized Finite Element Method for Multiscale Simulations: Armando Duarte (UIUC)

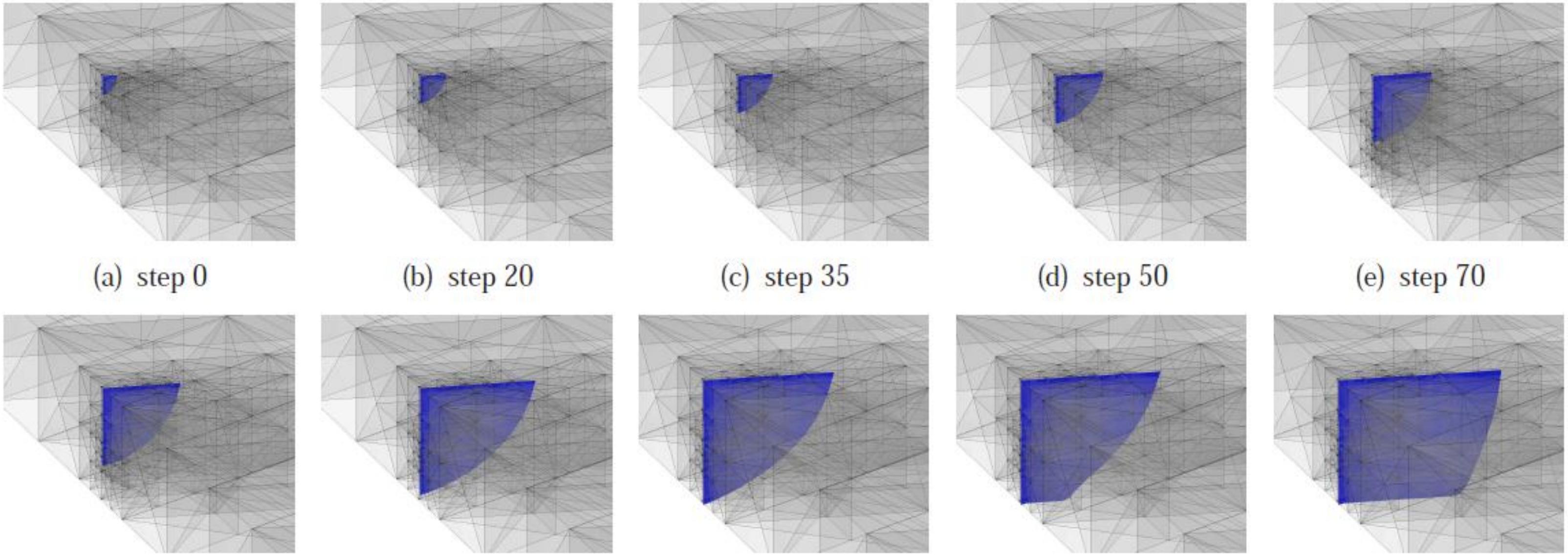
Extensions to Nonlinear Problems:



Key Properties:

- Uses available information at a simulation step to build approximation spaces for the next step
- Uses coarse FEM meshes; solution spaces of much reduced dimension than in the FEM
- Two-way information transfer between scales; account for interactions among scales

Example: Simulation of 3-D Propagating Cracks



(a) step 0 (b) step 20 (c) step 35 (d) step 50 (e) step 70

(f) step 85 (g) step 93 (h) step 103 (i) step 110 (j) step 146

- FAST: Coarse-scale model of much reduced dimension than FEM; Fine-Scale computations are intrinsically parallelizable; recycle coarse scale solution
- ACCURATE: Can deliver same accuracy as adaptive mesh refinement (AMR) on meshes with elements that are orders of magnitude larger than in the FEM
- STABLE: Uses single-field variational principles
- TRANSITION: Fully compatible with FEM

Uncertainty Quantification MURI
Broad MURI Objectives

- To develop rigorous **theory, algorithms and software** for UQ management in a computationally scalable way.

- Challenges include
  - proper formulation of stochastic models
  - high-dimensional problems
  - Proper numerics: efficiency, accuracy
  - Challenging application problems: stochastic multiscale problems
  - Need for new frameworks for dealing with model uncertainty, combining epistemic and aleatory uncertainties
  - Inverse Problems
  - Design and Control problems

Research Highlights

- **Mathematical Theory:** Quantization-renormalization of SPDEs; New evolution equations for joint-pdf of SPDEs; Nonlinear Malliavin calculus

- **Reduced Basis Methods (RBM):** Integral equations and multi-scattering problems; Robust design, parameter estimation, and model uncertainty

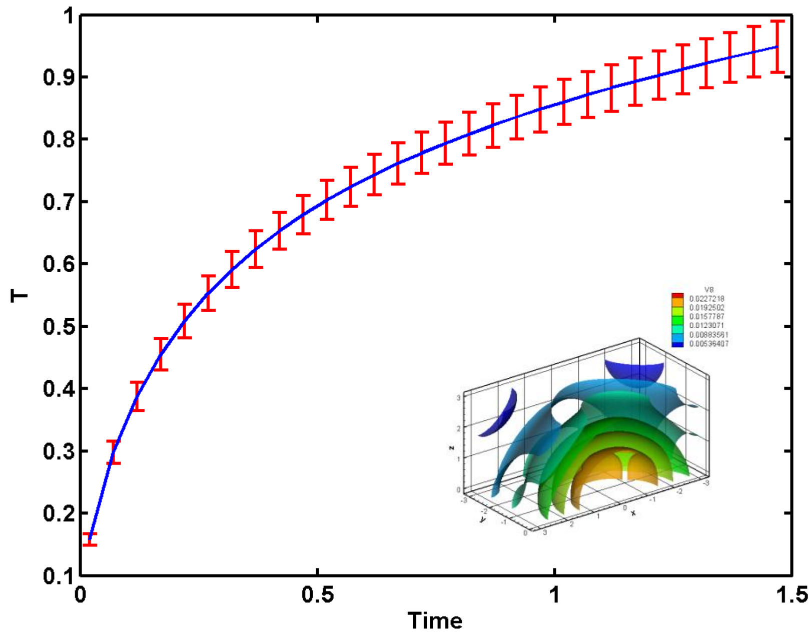
- **Adaptive ANOVA:** Convergence theory; Parameter compression and RBM; Fluid flows, porous media, multi-scattering

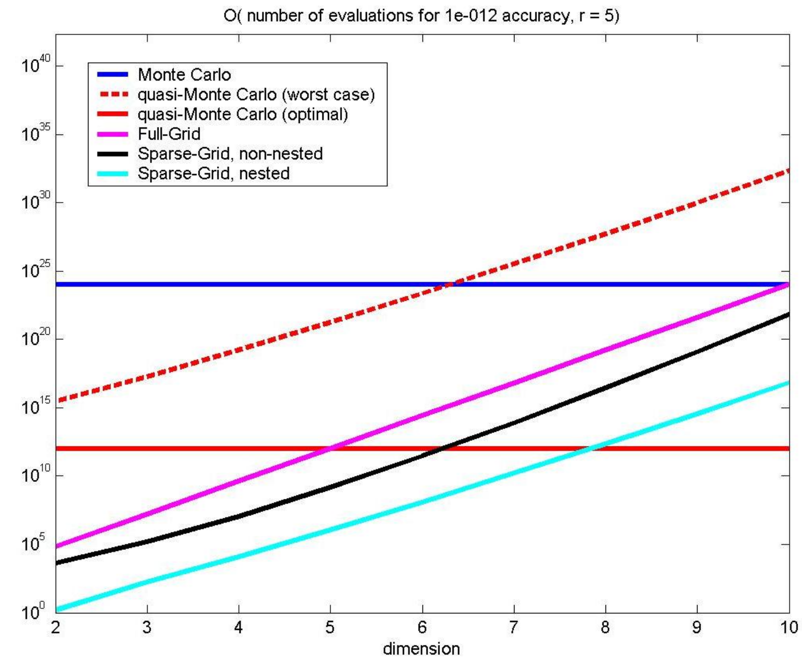
- **Bayesian Framework:** coarse-graining; Active learning + SPDEs; Adaptive SMC, dependent random variables, model uncertainty in inverse problems

- **Numerical SPDEs:** Data-driven stochastic multiscale method; Multiscale, multilevel MC, long-time integrators of SPDEs

- **Software:** MEPCM library; Reduced basis method libraries - RBOOMIT, RBAppMIT; Random poly-crystals - RPCrystal

New stochastic modeling methods are required for time-dependent and high-dimensional problems





- **Uncertainty increases in time**
- **Curse of dimensionality**

New Developments: Adaptive ANOVA, Multi-Level MC, New joint PDF Theory, Time-Dependent Chaos Basis, Quantization/Normalization

Main Result: New methods beat Stochastic Collocation (standard) by several orders of magnitude.

Adaptive ANOVA for 100-Dimensional Problems

- Hierarchical decomposition of a multidimensional function into combinations of functions of subgroups of its dimensions (allow only ν-body interactions)

$$
\begin{aligned}
\mathcal{I}_\mu f(x_1, x_2, \ldots, x_N) \quad = \\
\mathcal{I}_\mu f_0 + \sum_{j_1,(\nu=1)}^{N} \mathcal{I}_\mu f_{j_1}(x_{j_1}) + \sum_{j_1<j_2,(\nu=2)}^{N} \mathcal{I}_\mu f_{j_1,j_2}(x_{j_1}, x_{j_2}) + \\
\sum_{j_1<j_2<j_3,(\nu=3)}^{N} \mathcal{I}_\mu f_{j_1,j_2,j_3}(x_{j_1}, x_{j_2}, x_{j_3}) + \cdots \mathcal{I}_\mu f_{j_1,\ldots,j_N}(x_{j_1}, \cdots, x_{j_N})
\end{aligned}
$$

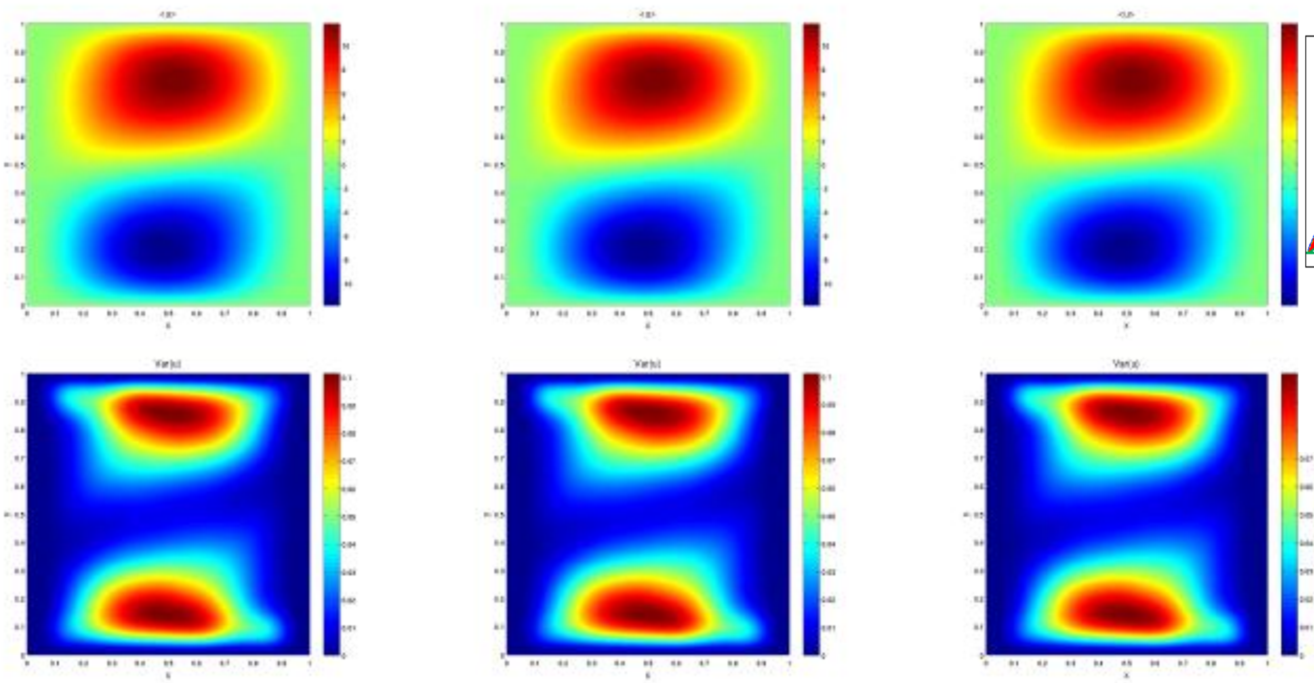
μ: **order of Polynomial Chaos approximation**

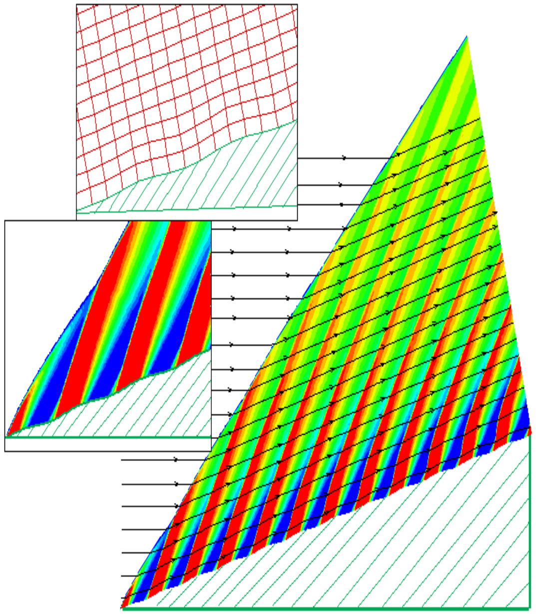
ν : **dimension of each sub-problem**

Adaptive ANOVA: 100-dimensional Flows

➢**Ref: Yang, Choi & Karniadakis, JCP, 2011**

Thermal convection in a closed cavity with random boundary conditions





V[u]: variance

MC (90,000 samples)

Sparse Grid Level 2 (#:18625)

ANOVA μ=2, ν=1 (#:193)

Bayesian Framework for UQ:

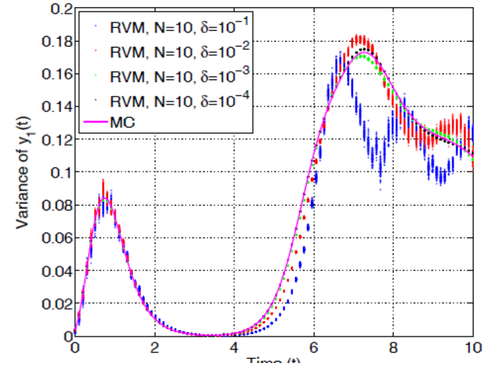
Zabaras(Cornell)

Builds surrogate surface

Informative data collection

Error bars for the statistics

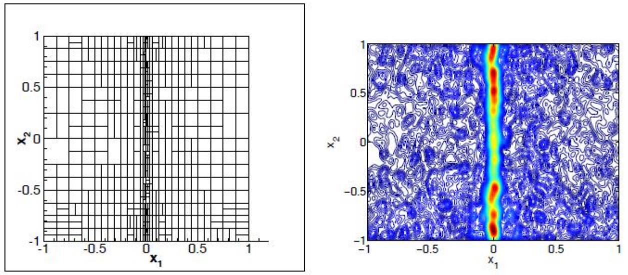
Bayesian Methods (GP, RVM, etc.)



Problem set up:

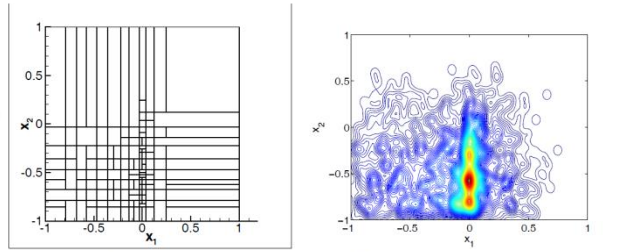
1. Deterministic (multiscale) solver
2. Limited data.
3. Stochastic discontinuities.
4. Multiple outputs

Hierarchical binary trees



(e) Elements: $\delta = 10^{-5}$

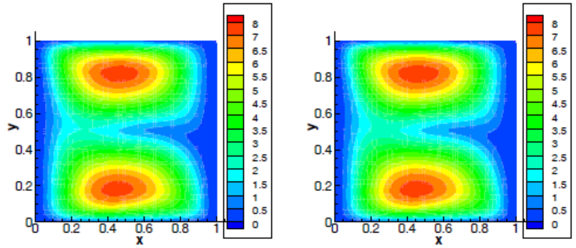
(f) Observed input: $\delta = 10^{-5}$



(a) Elements: $\delta = 10^{-4}$

(b) Observed input: $\delta = 10^{-4}$

Capturing correlations



(a) K=8, MGP ($N = 20, \delta = 10^{-3}$): std. of u

(b) K=8, MC: std. of u

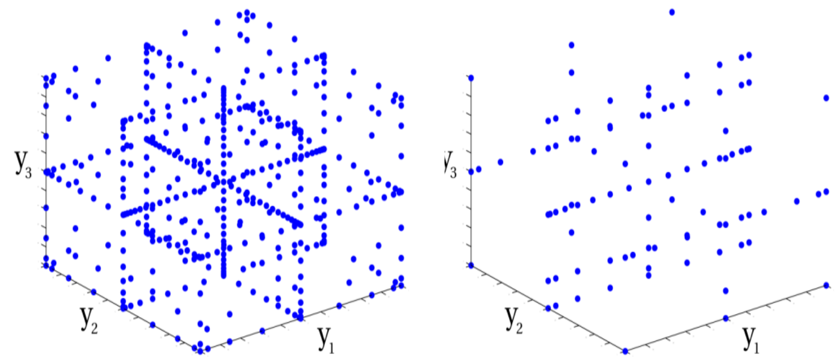
Bayesian Exploration Statistical Toolbox C++

"Designing the Next Generation Exascale Statistical and Uncertainty Quantification Tools"

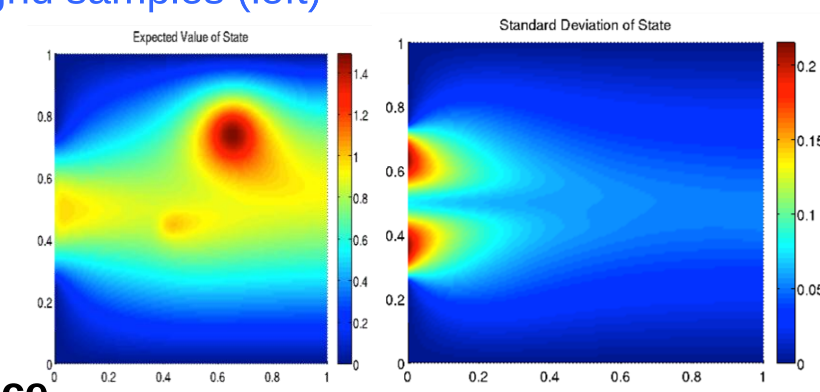
- **Objectives:**
  - High-dimensional, data-driven exploration of PDE-based engineering and science problems
  - Fast implementation and testing of novel statistical algorithms
- **Key ideas:**
  - **Modularity:**
  - **Efficiency/Scalability:**
- **Features:**
  - **Optimized templated versions of core statistical models**
  - **Data-based input modeling**
  - **Uncertainty propagation**
  - **Inverse problems**

Adaptive Methods for Stochastic PDE Constrained Optimization: M. Heinkenschloss (Rice)

- **Optimal control and design problems uncertain inputs.**
- **Proper incorporation of uncertainties decisions.**
- **Resulting optimization problems require 'sampling' of uncertainties and are expensive to solve. Expense increases with sample size.**
- **Developed optimization approach based on adaptive sparse grids:**
  - **Importance of the random inputs on optimization detected automatically.**
  - **Sampling is adjusted to keep number of PDE solves at minimum while ensuring convergence.**
  - **Implementation using Trilinos for parallelism.**
- **Adaptive sampling leads to reduction in computing time by a factor of 15 to 20.**



Adaptive sampling (right) substantially reduces sample size over classical sparse grid samples (left)



Source inversion problem. Expected value (left) and standard deviation (right) of PDE solution. Large STDEV near left bdry due to uncertain inflow.

Future Directions

- **Continued support of high-order methods in multiscale and multiphysics modeling, support in time-integration methods**
- **Continued emphasis on UQ and V&V**
  - **Numerical methods, Sampling methods, Design under Uncertainty**
- **Algorithms for multi-core platforms: GPU computing**
- **Emphasis on scalability of algorithms for ultra-parallel large scale computing**
- **Data-Driven Modeling and Computation**
  - **Combination of new estimation techniques with large scale computing: new ideas in data assimilation**
- **Understanding the impact of geometric discretization on the fidelity of the analysis and computation**